

Neutron Drops and Skyrme Energy-Density Functionals

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Abstract

The $J^\pi=0^+$ ground state of a drop of 8 neutrons and the lowest $1/2^-$ and $3/2^-$ states of 7-neutron drops, all in an external well, are computed accurately with variational and Green's function Monte Carlo methods for a Hamiltonian containing the Argonne v_{18} two-nucleon and Urbana IX three-nucleon potentials. These states are also calculated using Skyrme-type energy-density functionals. Commonly used functionals overestimate the central density of these drops and the spin-orbit splitting of 7-neutron drops. Improvements in the functionals are suggested.

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Properties of neutron matter are vitally important in determining the structure of neutron stars [1], and have a strong bearing on the energies of neutron-rich nuclei, and on the r-process in nucleosynthesis [2]. It is impossible to extrapolate available data on nuclei to the region of neutron matter with sufficient precision using effective interactions. Different effective interactions that fit the energies of laboratory nuclei rather well predict very different equations of state for neutron matter [1]. In contrast, it appears that modern calculations of neutron matter based on realistic models of nuclear forces are much more consistent with each other at densities $\rho \lesssim 0.16 \text{ fm}^{-3}$ [3], and therefore are presumably more reliable. The two-nucleon interaction in these realistic models is better determined from the scattering data in isospin $T=1$ states than that in $T=0$, and the uncertainties coming from three-nucleon forces and relativistic effects are also much smaller in neutron than in nuclear matter. Calculations of uniform neutron matter have provided important constraints on Skyrme-type effective interactions used to study neutron-rich systems. They do not, however, provide information on the strength of the spin-orbit interaction, nor on other terms sensitive to density gradients, both of which may affect significantly the predicted properties of drip-line nuclei and of neutron-star matter.

Ab initio calculations of finite nuclei, based on realistic models of nuclear forces, can provide the necessary additional information, but they are more challenging. Recently [4] the energies of nuclei with $A \leq 6$ have been calculated essentially exactly with the Green's function Monte Carlo (GFMC) method. Cluster variational Monte Carlo (CVMC) calculations have also been used to study ^{16}O [5] and the spin-orbit splitting (SOS) in ^{15}N [6]. In this letter we report GFMC and CVMC calculations of states of seven and eight neutrons bound in a weak external potential well using the new Argonne two-nucleon [7] and Urbana three-nucleon interactions used in Ref. [4]. These interactions accurately reproduce the available two-nucleon scattering data and binding energies of $A \leq 6$ nuclei. Neutron matter is not bound, therefore an external well (V_{ex}) is necessary to hold the neutrons together. We have used a Woods-Saxon well with $V_o = -20 \text{ MeV}$, $R = 3 \text{ fm}$, and $a = 0.65 \text{ fm}$, chosen such that with it alone only the single-neutron $1s$ state is bound at -5.73 MeV , while the $1p$ and higher

states are unbound. The investigated states of seven and eight neutrons are thus bound by both the well and the interaction between neutrons. We denote them by ${}^8\text{n}(J^\pi = 0^+)$ and ${}^7\text{n}(J^\pi = 1/2^- \text{ and } 3/2^-)$.

The present variational Monte Carlo (VMC) and GFMC calculations are simpler than those for nuclei [4] because all nucleons are neutrons. The wave function is represented by a vector function of \vec{R} ($\equiv \vec{r}_1, \vec{r}_2, \dots, \vec{r}_A$) with 2^A spin components specifying the spin direction of each neutron. The VMC and GFMC calculations use a simpler variational wave function than those of Refs [4,5]:

$$|\Psi_V\rangle = \left[S \prod_{i<j} (1 + U_{ij}) \right] \left[\prod_{i<j} f_c(r_{ij}) \right] |\Phi\rangle, \quad (1)$$

$$U_{ij} = u_\sigma(r_{ij}) \sigma_i \cdot \sigma_j + u_t(r_{ij}) S_{ij}. \quad (2)$$

Here S_{ij} denotes a symmetrized product, S_{ij} is the tensor operator, $f_c(r_{ij})$ is the Jastrow correlation, and $|\Phi\rangle$ is an antisymmetric shell model wave function. The three-body correlations commonly used in nuclear Ψ_V are omitted because they have little effect on the energies of low-density neutron systems, and the two-body spin-orbit correlations are discussed later along with an improved Ψ_V . The radial wave functions of the s- and p-orbitals in Φ and the correlation functions f_c , u_σ and u_t are determined variationally.

The GFMC calculations are carried out as described in Ref. [4] with a simpler Hamiltonian:

$$H = - \sum_i \frac{\hbar^2}{2m} \nabla_i^2 + \sum_i V_{ex}(i) + \sum_{i<j} v'_8(ij) + \sum_{i<j<k} V_{ijk}, \quad (3)$$

where the v'_8 does not contain L^2 or $(L \cdot S)^2$ terms; it equals the charge-symmetric part of the Argonne v_{18} interaction [7] in the 1S_0 and ${}^3P_{J=0,1,2}$ two-neutron states. The small difference between the full v_{18} and v'_8 is treated as a first-order perturbation, whose contribution to the calculated energies is < 0.2 MeV.

The calculated transient energies, $E(\tau)$,

$$E(\tau) = \langle \Psi_V | H e^{-(H-E_o)\tau} | \Psi_V \rangle / \langle \Psi_V | e^{-(H-E_o)\tau} | \Psi_V \rangle, \quad (4)$$

are shown in Fig.1. The $E(\tau \rightarrow \infty)$ converges to the lowest eigenvalue of the chosen J^π . In Fermi systems, the statistical error in $E(\tau)$ increases with τ as configurations diffuse across nodal surfaces of the wave function [9]. Due to the large number of nodal surfaces in the wave functions of ${}^7\text{n}$ and ${}^8\text{n}$ states, it is difficult to study their transient energy for values of $\tau > 0.04 \text{ MeV}^{-1}$. The average values of $E(\tau)$ for $\tau = 0.032, 0.036$ and 0.04 MeV^{-1} , denoted by \bar{E} , are shown by horizontal lines in Fig. 1. The $E(\tau)$ of the ${}^8\text{n}(0^+)$ and ${}^7\text{n}(1/2^-)$ states do not have much τ -dependence for $\tau > 0.015 \text{ MeV}^{-1}$, suggesting that their \bar{E} can be identified with the eigenvalues. In contrast, the $E(\tau)$ of the ${}^7\text{n}(3/2^-)$ state has more τ -dependence. Consequently, the eigenvalue of the lowest ${}^7\text{n}(3/2^-)$ state could be a little below its \bar{E} value. However, we will neglect that difference and regard it as our best estimate of the eigenvalue. The GFMC estimate of the density distribution of neutrons in the ${}^8\text{n}(0^+)$ drop is shown in Fig. 2. These results can be used to test the accuracy of the CVMC method and to further constrain the Skyrme type energy-density functionals used to study neutron-rich nuclei and neutron star crusts as discussed below.

The CVMC method and its modification for SOS are described in Refs. [5,6]. The present CVMC calculations are more accurate; they include contributions of all correlations and interactions up to five-body clusters. In contrast, in [5,6] contributions of only static correlations and interactions were calculated up to four-body clusters and the momentum-dependent terms were evaluated only at the two-body level. With the simpler Ψ_V given by Eq. (1), the 1- to 5-body cluster contributions to the energy of ${}^8\text{n}(0^+)$ state are respectively 12.9, -54.5, 11.1, -3.8, and 1.1 MeV, which sum up to -33.3(2) MeV. The $E(\tau = 0)$ is nothing but the variational energy calculated to all orders without cluster expansion. Its value of -33.7(1) MeV is very close to the CVMC result retaining up to five-body clusters. Note that even in this rather low-density system, the cluster expansion has a slow convergence and it appears necessary to include five-body cluster contributions to reduce the truncation error to $< 2\%$.

The simple Ψ_V (Eq. 1) is not very accurate; the energy obtained with it is $\sim 4 \text{ MeV}$ (or $\sim 11\%$) too large. In CVMC we use the more general variational wave functions of the

form:

$$|\Psi'_V\rangle = \left[1 + \sum_{i<j<k} U_{ijk}\right] \left[S \prod_{i<j} (1 + U_{ij})\right] \left[1 + \sum_{i<j} u_{L\cdot S}(r_{ij}) L_{ij} \cdot (\sigma_i + \sigma_j)\right] \left[\prod_{i<j} f_c(r_{ij})\right] |\Phi\rangle \quad (5)$$

where the three-body correlations, U_{ijk} , are of the kind used in Refs. [5,6] (note, however, that the commutator term is zero in pure neutron systems), and as before the U_{ij} contains spin and tensor terms. The energies obtained with the Ψ'_V variational wave functions are respectively -35.6(1), -31.2(1), -29.7(1) MeV for the ${}^8\text{n}(0^+)$, ${}^7\text{n}(\frac{1}{2}^-)$ and ${}^7\text{n}(\frac{3}{2}^-)$ states. They are only $\sim 4\%$ above the GFMC energies -37.6(3), -32.3(2) and -31.2(2) MeV. The CVMC calculations require about a factor of 25 less computer time than the GFMC, even allowing for the variational search. It is not difficult to reduce the statistical error in CVMC calculations to a fraction of one percent. Much of the improvement in Ψ'_V comes from the spin-orbit correlations omitted in the simpler Ψ_V . In the present GFMC calculations, the spin-orbit correlations are built in exactly via the propagation in imaginary time.

Fragmentation of the $p_{3/2}$ strength in ${}^{15}\text{N}$ results in the SOS of $p_{1/2}$ and $p_{3/2}$ quasi-hole states being ~ 0.6 MeV larger than the observed splitting between the lowest $3/2^-$ and $1/2^-$ states in ${}^{15}\text{N}$ [6,10]. If the $3/2^-$ hole strength in ${}^7\text{n}$ is similarly fragmented, the difference in the energies of lowest ${}^7\text{n}(1/2^-)$ and ${}^7\text{n}(3/2^-)$ states could be smaller than the SOS in ${}^7\text{n}$. If W denotes the energy width of the fragmentation, the GFMC transient energies, $E(\tau)$, for $\tau \geq 1/W$ will include fragmentation effects. Since W is expected to be only a few MeV, it is very unlikely that the present \bar{E} evaluated up to $\tau \sim 0.04$ has any fragmentation effects. The ${}^7\text{n}$ variational wave functions are constructed by removing an appropriate state from the $|\Phi\rangle$ and thus correspond to quasi-hole states. Presumably, they too do not contain any fragmentation effects. Hence, we identify the difference between the calculated energies of the ${}^7\text{n}(1/2^-)$ and $(3/2^-)$ states as the spin-orbit splitting. Its value is 1.1 ± 0.3 and 1.4 ± 0.1 MeV in the GFMC and CVMC calculations respectively.

The energies of uniform neutron matter calculated from several realistic models of nuclear forces were plotted in Ref. [1] and compared with the results of four energy-density

functionals (EDF) used for astrophysical investigations involving dense matter: (i) Skyrme 1' - Vautherin-Brink Skyrme model 1 [11] modified [12] to fit the neutron-matter $E(\rho)$ of Ref. [13]; (ii) SkM - Skyrme model M [14]; (iii) FPS - a generalized Skyrme model fitted approximately [15,1] to the nuclear- and neutron-matter energies of Ref. [16]; and (iv) FPS21 - a generalized Skyrme model [1] fitted accurately to results of Ref. [16]. These EDF's reproduce the ground-state energies of stable closed-shell nuclei rather accurately. The root mean square deviations $|\Delta E/E|$ between their prediction and experiment for ^{16}O , ^{40}Ca , ^{48}Ca , ^{56}Ni , ^{90}Zr , ^{114}Sn , ^{140}Ce , and ^{208}Pb are listed in Table I. This table also contains their predictions for the energy of the ^8n ground state and the ^7n and ^{15}N SOS. The results for the density distributions $\rho(r)$ of the $^8\text{n}(0^+)$ state are compared with the GFMC and CVMC $\rho(r)$ in Fig. 2.

In trying to learn from the departures of the EDF results for ^8n and ^7n from our benchmarks, we concentrate on the FPS21 effective interaction, since it gives the closest fit to the neutron-matter energies. Possible sources of difference include the fact that the neutron-matter energies used [16] date from an earlier period, whereas the benchmark results use newer interactions and more subtle computational techniques; also, and more importantly, the density-gradient terms in FPS21 are related to the effective-mass results [16] assuming a zero-range nucleon-nucleon interaction with no spin exchange. The latter simplification is common to all of the EDF's we consider and is not well justified. On the assumption that this is a contributor to the discrepancy, we have examined the effect of adding a term, $\frac{1}{2}\alpha(\rho_n)^\beta(\nabla\rho_n)^2$, to the FPS21 neutron EDF. The gradient term, $\frac{1}{2}\alpha(\rho_n + \rho_p)^\beta(\nabla\rho_n - \nabla\rho_p)^2$, reduces to the form used for neutron drops, and would give little contribution for $N \sim Z$ nuclei. However, in this work we have used it only for the neutron drops to avoid refitting the models to laboratory nuclei. Such a term can correct for the overbinding of $^8\text{n}(0^+)$, and also reduce the central neutron densities. We find that it cannot give good fits to these quantities simultaneously, however. For the two sets of coefficients $(\beta, \alpha) = (0, 150 \text{ MeV fm}^8)$ and $(2, 7 \times 10^4 \text{ MeV fm}^{14})$ the ground state energies of ^8n are -39.6MeV and -40.2MeV respectively, and the neutron density distributions are shown as curves A and B in Fig. 2.

The present CVMC and GFMC results clearly indicate that the SOS predicted by the unadjusted Skyrme models for ${}^7\text{n}$ is too large, while it is good for ${}^{15}\text{N}$. Relativistic mean-field models also predict a weaker spin-orbit potential in neutron-rich nuclei [17]. The neutron spin-orbit potential in these Skyrme models is of the form

$$V_{\ell s}^{(n)}(r) = W_{\ell s} \frac{1}{r} \frac{d}{dr} (\rho(r) + \rho_n(r)), \quad (6)$$

obtained by Vautherin and Brink [11] assuming that it originates from two-nucleon interactions in the triplet-P state. Here $\rho(r) = \rho_n(r) + \rho_p(r)$ and $W_{\ell s}$ is a constant determined from the SOS in laboratory nuclei like ${}^{15}\text{N}$, and listed in Table I. The form of this potential, proportional to a radial derivative of the densities, indicates that apart from other dependences, the SOS obtained with a given EDF will depend on the nucleon central densities given by that model. The two modified versions of FPS21 just described, for the same value $W_{\ell s} = 110\text{MeV}$ used in Table I, each give a SOS in ${}^7\text{n}$ of 2.2 MeV. The reduction from the value of 3 MeV for unmodified FPS21 occurs because of the reduced central densities induced by the extra gradient term. The SOS in these modified models is still about double the value predicted by CVMC and GFMC, however.

As discussed in Ref. [6], more than half the SOS in ${}^{15}\text{N}$ comes from three-nucleon contributions involving either two neutrons and a proton or vice-versa. In contrast, the three-body interaction and clusters give a very small contribution to the SOS in ${}^7\text{n}$ in CVMC calculations. This suggests adding terms to the EDF that will produce a spin-orbit potential:

$$V_{\ell s}^{(n)}(r) = W_{\ell s}^{(2)} \frac{1}{r} \frac{d}{dr} (\rho(r) + \rho_n(r)) + W_{1,\ell s}^{(3)} \frac{1}{r} \frac{d}{dr} (\rho_n(r) \rho_p(r)) + W_{2,\ell s}^{(3)} \frac{1}{r} \frac{d}{dr} (\rho_p(r))^2 \quad (7)$$

having separate two- and three-body contributions. The $(\rho_n(r))^2$ term is omitted because three-neutron clusters seem to give negligible $V_{\ell s}^{(n)}(r)$. In neutron drops only the two-body $W_{\ell s}^{(2)}$ contributes, while in $N \sim Z$ nuclei, like ${}^{15}\text{N}$, $\rho_n(r) \rho_p(r) \sim \rho_p(r)^2$ and the sum $W_{\ell s}^{(3)} = W_{1,\ell s}^{(3)} + W_{2,\ell s}^{(3)}$ is the only relevant new parameter.

With this modification to the spin-orbit interaction, and the FPS21 parameterization for the central interaction (including the gradient term for the neutron drops but not for ${}^{15}\text{N}$),

we can fit the spin-orbit splittings of ^{15}N and ^7n exactly, using the parameter values $W_{\ell s}^{(2)} = 61 \text{ MeV fm}^5$ and $W_{\ell s}^{(3)} = 745 \text{ MeV fm}^8$. The spin-orbit splittings in the eight closed-shell nuclei mentioned earlier are modified only slightly, a not unexpected result in view of their relatively small values of neutron excess

In conclusion, we have made the first exact microscopic calculations of neutron drops in an external potential well. Our results suggest that the commonly used EDF's need modification in order to describe accurately neutron-rich nuclei. It appears that they predict neutron drops which are too dense and have too large a spin-orbit splitting. Additional density gradient terms need to be considered and the parameterization of the Skyrme $V_{\ell s}$ must be modified to include three-body contributions. Our GFMC results also show that the CVMC using the improved Ψ'_V , with two-neutron spin-orbit correlations gives fairly accurate results. We plan to use CVMC to calculate the properties of larger neutron drops. This, together with data from stable nuclei, will provide a larger database for fitting a Skyrme EDF for studies of stable nuclei, neutron rich nuclei, and the surface of neutron stars.

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TABLES

TABLE I. Comparison of microscopic and Skyrme-model energies.

	$^8\text{n}(0^+)$	^7n SOS	Magic Nuclei	^{15}N SOS ^a	$W_{\ell s}$
	MeV	MeV	$ \Delta E/E _{rms}\%$	MeV	MeV ⁵
GFMC	-37.6(3)	1.1(3)			
CVMC	-35.5(1)	1.4(1)	—	6.1 ^b	
SkM	-47.4	3.0	1.1	6.3	130
FPS-21	-42.2	3.0	1.1	6.7	110
Skyrme 1'	-38.7	2.9	1.8	6.9	120
FPS	-32.5	3.5	1.2	6.7	110

^aExperimental value 6.9 MeV deduced in Ref. [6].

^bWith Argonne v_{14} , Ref. [6].

FIGURES

FIG. 1. The transient energy $E(\tau)$ for the GFMC calculations of ${}^8\text{n}(0^+)$ and ${}^7\text{n}(1/2^-)$ and $3/2^-)$ as a function of the imaginary time τ .

FIG. 2. Neutron density distribution for ${}^8\text{n}$, according to methods described in the text. The curves labeled A and B come from modified versions of the effective interaction FPS21.



